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ON DIFFERENTIATING
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Report #31

*On Differentiating the Probability of Error
In The Multipopulation Feature Selection Problem, II*

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ABSTRACT

In this note we give a necessary and sufficient condition for the Gateaux differentiability of the probability of misclassification as a function of a feature selection matrix B , assuming a maximum likelihood classifier and normally distributed populations. It is also shown that if the probability of error has a local minimum at B then it is differentiable at B .

On Differentiating the Probability of Error in
the Multipopulation Feature Selection Problem, II.

1. Introduction.

Let π_1, \dots, π_m be populations in R^n with a priori probabilities $\alpha_1, \dots, \alpha_m$ and multivariate normal conditional density functions,

$$P_i(x) = \frac{1}{(2\pi)^{n/2} |\Sigma_i|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu_i)^T \Sigma_i^{-1} (x-\mu_i)\right].$$

$i = 1, \dots, m$. If B is a $k \times n$ matrix of rank k then the transformed conditional densities are, for $y \in R^k$,

$$P_i(y, B) = \frac{1}{(2\pi)^{k/2} |B\Sigma_i B^T|^{1/2}} \exp\left[-\frac{1}{2}(y-B\mu_i)^T (B\Sigma_i B^T)^{-1} (y-B\mu_i)\right].$$

Let $g(B)$ denote the probability of misclassifying an observation $x \in R^n$ using the Bayes optimal classifier: classify x in π_i if $\alpha_i P_i(Bx, B) \geq \alpha_j P_j(Bx, B)$ for each $j = 1, \dots, m$. Then $g(B) = 1 - h(B)$, where

$$h(B) = \int_{R^k} \max_{1 \leq i \leq m} \alpha_i P_i(y, B) dy.$$

is the probability of correct classification.

If the transformed probability of error is to be used as a feature selection criterion we require a method for obtaining a $k \times n$ matrix B_0 of rank k which minimizes $g(B)$. If B_0 minimizes $g(B)$ then the Gateaux differential, [2,p.178],

$$\delta g(B_0; C) = \lim_{s \rightarrow 0} \frac{g(B_0 + sC) - g(B_0)}{s}$$

vanishes for all $k \times n$ matrices C for which it exists. If $\delta g(B_0; C)$ exists for all $k \times n$ matrices C , then g is said to be Gateaux differentiable at B_0 . Thus it is desirable to have necessary and sufficient conditions for Gateaux differentiability of g as well as a formula for $\delta g(B; C)$.

2. Main Results.

For a given $k \times n$ matrix B partition the set $\{\alpha_i P_i(x)\}_{i=1}^m$ into disjoint sets

$$S_1 = \{\alpha_{11} P_{11}(x), \alpha_{12} P_{12}(x), \dots, \alpha_{1n_1} P_{1n_1}(x)\}$$

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$$S_r = \{\alpha_{r1} P_{r1}(x), \alpha_{r2} P_{r2}(x), \dots, \alpha_{rn_r} P_{rn_r}(x)\}$$

where the S_q are defined by

$$\alpha_{qj} P_{qj}(y, B) \equiv \alpha_{qi} P_{qi}(y, B) \quad 1 \leq i, j \leq n_q$$

$$\alpha_{qj} P_{qj}(y, B) \neq \alpha_{\ell i} P_{\ell i}(y, B) \quad q \neq \ell$$

For $\ell = 1, \dots, r$ let

$$R_\ell = \{y \in R^k \mid \alpha_{\ell 1} P_{\ell 1}(y, B) > \alpha_{k1} P_{k1}(y, B), \quad k \neq \ell\}.$$

The R_ℓ are disjoint open sets which cover R^k except for a set M of measure zero.

For a given $k \times n$ matrix C write $P_{ij}(y, s)$ for $P_{ij}(y, B+sC)$ and $h(s)$ for $h(B+sC)$. That is, $h(s) = \int_{R^k} \max_{i,j} \alpha_{ij} P_{ij}(y, s) dy$.

Theorem 1: h is Gateaux differentiable at B if and only if for each ℓ such that $R_\ell \neq \emptyset$, $\mu_{\ell i} = \mu_{\ell j}$ and $\sum_{\ell i} B^T = \sum_{\ell j} B^T$ for each $i, j \leq n_\ell$.

Proof: By repeating some of the members of the S_q 's if necessary, we can assume $n_1 = n_2 = \dots = n_r = n_0$. Thus

$$h(s) = \int_{R^k} \max_{1 \leq j \leq n_0} \max_{1 \leq i \leq r} \alpha_{ij} P_{ij}(y, s) dy$$

$$\int_{R^k} \max_{1 \leq j \leq n_0} f_j(y, s) dy,$$

where $f_j(y, s) = \max_{1 \leq i \leq r} \alpha_{ij} P_{ij}(y, s)$

The $f_j(y, s)$ have the properties:

$$1) f_1(y, 0) \equiv f_2(y, 0) \equiv \dots \equiv f_{n_0}(y, 0)$$

and

2) $\frac{\partial f_j}{\partial s}(y, 0)$ is defined for all $y \notin M$, $j = 1, \dots, n_0$. By an argument in [3], it can be shown that for sufficiently small $|s|$, the difference quotients

$$\frac{f_j(y, s) - f_j(y, 0)}{s}$$

are bounded by an integrable function $\beta(y)$ for $y \notin M$. Hence, for $s > 0$,

$$\begin{aligned} \frac{h(s) - h(0)}{s} &= \int_{R^k} \frac{1}{s} [\max_{j \leq n_0} f_j(y, s) - \max_{j \leq n_0} f_j(y, 0)] dy \\ &= \int_{R^k} \frac{1}{s} \max_{j \leq n_0} [f_j(y, s) - f_j(y, 0)] dy \\ &= \int_{R^k} \max_{j \leq n_0} \frac{f_j(y, s) - f_j(y, 0)}{s} dy \\ &\rightarrow \int_{R^k} \max_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) dy \end{aligned}$$

as $s \rightarrow 0+$. On the other hand, for $s < 0$,

$$\begin{aligned} \frac{h(s) - h(0)}{s} &= \int_{R^k} \min_{j \leq n_0} \frac{f_j(y, s) - f_j(y, 0)}{s} dy \\ &\rightarrow \int_{R^k} \min_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) dy. \end{aligned}$$

as $s \rightarrow 0^-$. Thus the Gateaux differential $h'(0)$ exists if and only if

$$\max_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) = \min_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) \quad \text{a.e.}$$

That is, if and only if

$$\frac{\partial f_j}{\partial s}(y, 0) = \frac{\partial f_i}{\partial s}(y, 0) \quad \text{a.e.}$$

for all $i, j \leq n_0$. For $y \in R^\ell$ it is readily verified that

$$\frac{\partial f_i}{\partial s}(y, 0) = \alpha_{\ell i} \frac{\partial P_{\ell i}}{\partial s}(y, 0).$$

Hence, $h'(0)$ exists if and only if

$$\alpha_{\ell i} \frac{\partial P_{\ell i}}{\partial s}(y, 0) = \alpha_{\ell j} \frac{\partial P_{\ell j}}{\partial s}(y, 0)$$

for $i, j \leq n_0$, almost all $y \in R^\ell$, $\ell = 1, \dots, r$.

It is shown in [1], that

$$\begin{aligned} \alpha_{\ell j} \frac{\partial P_{\ell j}}{\partial s}(y, 0) &= \alpha_{\ell j} P_{\ell j}(y, 0) \{ (y - B\mu_{\ell j})^T (B\Sigma_{\ell j} B^T)^{-1} \\ &\quad [C\mu_{\ell j} + C\Sigma_{\ell j} B^T (B\Sigma_{\ell j} B^T)^{-1} (y - B\mu_{\ell j})] \\ &\quad - \text{tr}[C\Sigma_{\ell j} B^T (B\Sigma_{\ell j} B^T)^{-1}] \}. \end{aligned}$$

Since $B\mu_{\ell j} = B\mu_{\ell i}$, $B\Sigma_{\ell j}B^T = B\Sigma_{\ell i}B^T$, $\alpha_{\ell j} = \alpha_{\ell i}$,

$$\alpha_{\ell j} \frac{\partial P_{\ell j}}{\partial s}(y, o) = \alpha_{\ell i} P_{\ell i}(y, o) \{(y - B\mu_{\ell i})^T (B\Sigma_{\ell i}B^T)^{-1}$$

$$[C\mu_{\ell j} + C\Sigma_{\ell j}B^T(B\Sigma_{\ell i}B^T)^{-1}(y - B\mu_{\ell i})]$$

$$- \text{tr}[C\Sigma_{\ell j}B^T(B\Sigma_{\ell i}B^T)^{-1}]\}.$$

If $R_\ell \neq \emptyset$, then R_ℓ has positive measure. Thus it is easily seen that if $R_\ell \neq \emptyset$,

$$\alpha_{\ell i} \frac{\partial P_{\ell i}}{\partial s}(y, o) = \alpha_{\ell j} \frac{\partial P_{\ell j}}{\partial s}(y, o) \quad \text{a.e. in } R_\ell$$

if and only if $C\mu_{\ell j} = C\mu_{\ell i}$, $C\Sigma_{\ell j}B^T = C\Sigma_{\ell i}B^T$ for all $i, j \leq n_o$. Thus h is Gateaux differentiable at B if and only if $\mu_{\ell i} = \mu_{\ell j}$, $\Sigma_{\ell i}B^T = \Sigma_{\ell j}B^T$ $\forall i, j \leq n_o$, $\forall \ell$ such that $R_\ell \neq \emptyset$. This concludes the proof.

It is clear that if h is Gateaux differentiable at B , then

$$\delta h(B:C) = \sum_{i=1}^r \alpha_{i1} \int_{R_i} \delta P_{i1}(y, B:C) dy$$

Thus the Gateaux differential of the probability of error is

$$\delta g(B:C) = - \sum_{i=1}^r \alpha_{i1} \int_{R_i} \delta P_{i1}(y, B:C) dy.$$

Theorem 2: If h has a local maximum at B , then h is Gateaux differentiable at B .

Proof: It is evident from the proof of Theorem 1 that for any $k \times n$ matrix C ,

$$\begin{aligned} \limsup_{s \rightarrow 0} \frac{h(B+sC) - h(B)}{s} &= \lim_{s \rightarrow 0^+} \frac{h(B+sC) - h(B)}{s} \\ &= \int_{R^k} \max_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) dy \end{aligned}$$

and

$$\begin{aligned} \liminf_{s \rightarrow 0} \frac{h(B+sC) - h(B)}{s} &= \lim_{s \rightarrow 0^-} \frac{h(B+sC) - h(B)}{s} \\ &= \int_{R^k} \min_{j \leq n_0} \frac{\partial f_j}{\partial s}(y, 0) dy. \end{aligned}$$

If h has a maximum at B , then since $\lim_{s \rightarrow 0^-} \frac{h(B+sC) - h(B)}{s}$ exists,

$$\begin{aligned} \limsup_{s \rightarrow 0} \frac{h(B+sC) - h(B)}{s} &= \lim_{s \rightarrow 0^-} \frac{h(B+sC) - h(B)}{s} \\ &= \liminf_{s \rightarrow 0} \frac{h(B+sC) - h(B)}{s} \end{aligned}$$

Thus h is Gateaux differentiable at B . Q.E.D.

3. Concluding Remarks.

The meaning of the necessary and sufficient condition for differentiability of $g(B)$ becomes a little more obvious when it is applied to the two population problem. Let π_1 and π_2 be normally distributed populations in R^n with class statistics $\alpha_1, \mu_1, \Sigma_1$ and $\alpha_2, \mu_2, \Sigma_2$, respectively.

Case 1: $\alpha_1 \neq \alpha_2$. Then $g(B)$ is differentiable for all B .

Case 2: $\alpha_1 = \alpha_2, \mu_1 \neq \mu_2$. Then g is differentiable at B if and only if $B\mu_1 \neq B\mu_2$ or $B\Sigma_1B^T \neq B\Sigma_2B^T$.

Case 3: $\alpha_1 = \alpha_2, \mu_1 = \mu_2, \Sigma_1 - \Sigma_2$ is invertible. Then g is differentiable at B if and only if $B\Sigma_1B^T \neq B\Sigma_2B^T$.

Case 4: $\alpha_1 = \alpha_2, \mu_1 = \mu_2, \Sigma_1 - \Sigma_2$ is not invertible. Then g is differentiable at B if and only if $B\Sigma_1B^T \neq B\Sigma_2B^T$ or $\Sigma_1B^T = \Sigma_2B^T$.

As a special case of Case 4, we have the degenerate case in which the class statistics for π_1 and π_2 are the same. Then g is differentiable for all B and has derivative 0. Finally, we remark that it is mistakenly asserted in [3] that the condition $\alpha_i P_i(y, B) \neq \alpha_j P_j(y, B)$ is necessary as well as sufficient for differentiability of $g(B)$. As the analysis above shows, this is not even true in the two population problem.

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